Static and dynamic image potential for tunneling into a Luttinger liquid

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We study electron tunneling from a tip or a lead into an interacting quantum wire described by Luttinger liquid theory. Within a WKB-type approach, the Coulomb interaction between the wire and the tunneling electrons, as well as the finite traversal time are taken into account. Although the static image potential is only logarithmically suppressed against the bare Coulomb interaction, the dynamic image potential is not strong enough to alter power-law exponents entering the tunneling density of states.

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One-dimensional (1D) quantum wires (QWs) are at the focal point of current activities in condensed-matter physics. Fabrication advances in semiconductor heterostructures[1] and carbon nanotubes[2] allow the systematic study of phenomena arising only in one dimension. In particular, the physics of 1D nanowires is intimately connected with the concept of a Luttinger liquid (LL), exhibiting spin-charge separation, suppression of the tunneling density of states (TDOS), and interaction dependent power-laws in transport properties.[3,4] For nanotubes, the theoretically predicted[5] LL behavior has been convincingly established in several recent experiments.[6] Of particular importance was the measurement of the TDOS power-law exponent α, which provides information about the dimensionless interaction strength parameter g of the LL (where $0 < g \leq 1$). The TDOS can be obtained, e.g. from the tunneling current measured via weakly attached metallic leads. Another possibility is to use a scanning tunneling microscopy (STM) tip. Apart from the resolution of atomic and electronic properties of individual nanotubes successfully achieved in recent STM experiments,[7–9] a detailed analysis of nonlinear current-voltage curves in the spectroscopy (STS) mode would allow to extract the TDOS exponent.

So far in all theoretical studies of tunneling into a LL, it has tacitly been assumed that the electrons tunneling into the correlated fermion liquid do not modify the effective TDOS. Conventional treatments[10] employ the tunneling Hamiltonian and thereby assume the traversal time of tunneling[11] to be infinitely short. In addition, the interaction between the tunneling electron and the LL electrons is neglected. Given these two assumptions, the TDOS is indeed an intrinsic property of the LL with a power-law dependence on energy, $\rho(\epsilon) \propto \epsilon^{\alpha}$, for $\epsilon \to 0$, so that α depends only on g. (For clarity, we focus on the case of bulk tunneling at zero temperature throughout this paper.) For an STS experiment, such a calculation predicts that the measured differential conductance is proportional to the TDOS,[12] and hence the exponent α can be extracted from experimental data. A similar reasoning has been employed to understand the data in Ref. 6, where electron tunneling between metallic leads and a nanotube was important.

Here we address the question of *whether this measured exponent really characterizes the unperturbed LL*, or whether it is affected by the dynamics and charge of the tunneling particle. To that end, we take into account correlations both within the QW and between the QW and the tunneling electron, as well as a finite traversal time. Our main findings are as follows: Although the *static* image potential experienced by the tunneling electron is very strong, dynamical effects turn out to be of crucial importance. Within the framework of a semiclassical theory related to Nazarov's tunnel junction theory,[13] the low-energy power-law exponent of the TDOS is governed solely by intrinsic LL properties. Thereby we provide the *a posteriori* justification for the (previously assumed) connection linking the (observable) value of α and the interaction parameter g. Since spin and charge are decoupled in a LL, we study only the spinless single-channel case, with the same conclusions applying to spin-$\frac{1}{2}$ electrons or nanotubes.

For the case of tunneling from an STM tip into the QW, the relevant geometry is depicted in Figure 1. We consider a clean and very long ($L \to \infty$) QW, and mainly focus on an interaction potential of the form

$$V(x,y) = \frac{1}{\sqrt{x^2 + (D-y)^2 + a^2}} \,, \tag{1}$$

where a is the lattice constant of the QW. For $y = D$, this describes the intra-wire interaction responsible for the LL state, while for $0 < y < D$, it gives the interaction between the wire electrons and the tunneling electron at $x = 0$ (see below). The one-sided Fourier transform of Eq. (1) is

$$\tilde{V}(q,y) = 2K_0\left(|q|\sqrt{(D-y)^2 + a^2}\right) \,, \tag{2}$$

with the modified Bessel function K_0. When using Eq. (1), one neglects or crudely approximates several important effects, e.g. screening due to the tip, or the orbital structure of both tip and quantum wire (see, e.g. Ref. 9). However, our qualitative findings concerning the connection between α and g are expected to hold quite generally. In addition to the model potential (1), these findings can

be made rigorous for a general class of separable potentials.

Tunneling out of the tip (or lead) proceeds from the ground state with energy E_0' into the LL ground state with energy E_0, and is usually described in terms of a simple tunneling Hamiltonian,

$$H_T = T\Psi^\dagger(0)c_0 + \text{h.c.}\ , \tag{3}$$

where c_0 annihilates an electron in a state at the center of the tip and $\Psi^\dagger(0)$ creates an electron at $x=0$ in the LL. If the tunneling matrix element T is small, H_T can be treated as a perturbation to $H'+H$, where H' describes the electrons in the tip and H denotes the Hamiltonian of the LL. More specifically, the perturbative treatment is appropriate when the tunneling resistance is large compared to h/e^2. Then the tunneling rate Γ can be calculated with the aid of Fermi's golden rule. Labeling states in the tip by $|\nu\rangle$ and states in the LL by $|n\rangle$, the tunneling rate is (we put $\hbar=1$)

$$\Gamma = 2\pi T^2 \sum_{\nu,n} |\langle \nu,n|\Psi^\dagger(0)c_0|0,0\rangle|^2 \delta(E_0'+E_0-E_\nu'-E_n)\ ,$$

where $|0,0\rangle$ denotes the ground state in the absence of tunneling. Using the identity

$$\delta(E_0'+E_0-E_\nu'-E_n) = \int d\epsilon\ \delta(E_0+\epsilon-E_n)\delta(E_0'-\epsilon-E_\nu')\ ,$$

the rate may be written as

$$\Gamma = 2\pi T^2 \int_0^{eV} d\epsilon\ \rho(\epsilon)\rho'(eV-\epsilon)\ . \tag{4}$$

Here the TDOS for adding an electron with energy $\mu+\epsilon$ to the LL is

$$\rho(\epsilon) = \sum_n |\langle n|\Psi^\dagger(0)|0\rangle|^2 \delta(E_0+\mu+\epsilon-E_n)\ , \tag{5}$$

where the electrochemical potential μ is the minimal energy required to add an electron. Furthermore,

$$\rho'(\epsilon') = \sum_\nu |\langle \nu|c_0|0\rangle|^2 \delta(E_0'-\mu'+\epsilon'-E_\nu') \tag{6}$$

is the DOS for removing an electron from the tip/lead with energy $\mu'-\epsilon'$. Now $\rho(\epsilon)$ and $\rho'(\epsilon)$ are nonvanishing only for $\epsilon>0$, and $\mu'-\mu=eV$ determines the applied voltage. With these definitions we readily obtain Eq. (4). In a metallic lead, the DOS $\rho'(\epsilon)$ is essentially constant, while for an STM tip, we expect pronounced peaks reflecting the discrete level structure. In the latter case, Eq. (4) reproduces the rate from an STM tip into a metal first obtained by Tersoff and Hamann.[12]

To determine $\rho(\epsilon)$ explicitly, we write

$$\begin{aligned}\rho(\epsilon) &= \frac{\mathrm{Re}}{\pi}\int_0^\infty dt\ \sum_n \langle 0|\Psi(0)|n\rangle\langle n|\Psi^\dagger(0)|0\rangle e^{i(E_0+\mu+\epsilon-E_n)t} \\ &= \frac{\mathrm{Re}}{\pi}\int_0^\infty dt\ G_0(t)e^{i(\mu+\epsilon)t}\ ,\end{aligned} \tag{7}$$

with the single-electron Greens function ($t>0$) for an electron at position $x=0$ in the ground state, $G_0(t) = \langle\Psi(0,t)\Psi^\dagger(0,0)\rangle$. To evaluate $G_0(t)$, standard bosonization methods[3,4] can be applied. The kinetic part of the Hamiltonian is

$$H_0 = \frac{v_F}{2}\int dx\left[(\partial_x\vartheta)^2+(\partial_x\varphi)^2\right] + \mu\hat{N}\ .$$

Here v_F is the Fermi velocity, $\hat{N}$ the particle number operator, and $\vartheta(x)$ is conjugate to the phase field $\varphi(x)$ describing the plasmon excitations in the wire. The intra-wire interaction part is $H_V = \frac{1}{2}\int dx\,dx'\ n(x)V(x-x',D)n(x')$ with the electron charge density $n(x) = -e\pi^{-1/2}\partial_x\varphi$. (The LL model appropriate for the low energy sector follows by effectively using a local interaction, $V(x,D)=V_0\delta(x)$.) By virtue of a Bogoliubov transformation, $H=H_0+H_V$ can easily be diagonalized. With bosonic operators $b_q^{(\dagger)}$, the phase field $\varphi(x)$ reads[4]

$$\varphi(x) = i\sum_{q\neq0}\left(\frac{g(q)}{2L|q|}\right)^{1/2}\exp(-iqx)\,\mathrm{sgn}(q)\,[b_q^\dagger+b_{-q}]\ , \tag{8}$$

with the q-dependent interaction parameter [where $g=g(q=2\pi/L)$]

$$g(q) = [1+e^2\tilde{V}(q,D)/\pi v_F]^{-1/2} = g(-q)\ . \tag{9}$$

We then arrive at

$$H = \sum_{q\neq0}\omega_q b_q^\dagger b_q + \mu\hat{N}\ , \tag{10}$$

with the plasmon dispersion relation $\omega_q = v_F|q|/g(q)$. In terms of the chiral (right- or left-moving) phase fields ($p=R/L=\pm$),

$$\phi_p(x) = [p\varphi(x)+\vartheta(x)]/\sqrt{4\pi}\ , \tag{11}$$

the bosonized electron operator at $x=0$ is $\Psi(0,t)\propto\sum_{p=\pm}\exp[2\pi i\phi_p(0,t)]$, implying[3,4]

$$G_0(t)\propto t^{-(g+g^{-1})/2}\ e^{-i\mu t}$$

at long times. Hence one obtains the well-known exponent $\alpha=(g+g^{-1}-2)/2$ governing the bulk TDOS.

Let us now look at the *static image potential* experienced by an electron with charge $-e$ held fixed at position $x=0$ and $0<y<D$ due to its interaction with the QW electrons, $H_I = -e\int dx\ n(x)V(x,y) = -e\phi(y)$. Using Eq. (8), we get the fluctuating field

$$\phi(y,t) = \sum_{q\neq0}\lambda_q(y)\left(b_q^\dagger(t)+b_{-q}(t)\right) \tag{12}$$

with couplings $\lambda_q(y) = -e[g(q)|q|/2\pi L]^{1/2}\,\tilde{V}(q,y)$. Next we shift the bosonic operators,[14] $B_q = b_q - e\lambda_q(y)/\omega_q$, whence

$$H = \sum_{q\neq 0} \omega_q B_q^\dagger B_q + \mu\hat{N} + V_{im}(y) \ . \tag{13}$$

Here the static image potential

$$V_{im}(y) = -e^2 \sum_{q\neq 0} \lambda_q^2(y)/\omega_q \tag{14}$$

describes the energy gained by the plasmons relaxing to their equilibrium state in the presence of the additional electron. For the unscreened interaction (1), one has $g(q) = [1 + \xi K_0(|q|a)]^{-1/2}$ with the dimensionless parameter $\xi = 2e^2/\pi v_F$. Then the image potential (14) for $(D-y) \gg a$ reads

$$V_{im}(y) = -\frac{2e^2/\pi}{(D-y)\{\ln[(D-y)/a] + 1/\xi\}} \ .$$

Therefore the static image potential is *only logarithmically suppressed* against the bare Coulomb interaction, and hence is very strong.

Next we turn to dynamical effects due to tunneling. We envision the latter as penetration through a rectangular barrier of width D. If the barrier is sufficiently thick and its transparency low, the main contribution to the tunnel current comes from electrons with momenta perpendicular to the QW. Therefore we effectively obtain a 1D Schrödinger equation for the underbarrier motion $\psi(y,t)$ of the tunneling electron $(0 < y < D)$,

$$i\partial_t \psi(y,t) = [-(2m)^{-1}\partial_y^2 + \mu' + U - e\phi(y,t)]\psi(y,t) \ , \tag{15}$$

where U is the work function of the tip/lead. In the absence of $\phi(y,t)$, the solution for an electron at energy μ' reads $\psi(y,t) \propto e^{-i\mu' t - mvy}$, where $v = \sqrt{2U/m}$ is an effective velocity related to the traversal time D/v. Under the WKB approximation, the dominant effect of the potential ϕ can be incorporated as additional phase factor,[13]

$$\psi(y,t) \propto e^{-i\mu' t - mvy - i\theta(y,t)} \ . \tag{16}$$

Linearizing the resulting WKB equation gives for $|\phi(y,t)| \ll U$:

$$\partial_t \theta + iv\partial_y \theta = -e\phi(y,t) \ , \tag{17}$$

supplemented by the boundary condition $\theta(0,t) = 0$. This equation can be solved separately for each bosonic mode using the ansatz

$$\theta(y,t) = \sum_{q\neq 0} \left[w(y,\omega_q) b_{-q}(t) + \tilde{w}(y,\omega_q) b_q^\dagger(t) \right] \ .$$

From Eq. (17) and $b_q(t) = b_q e^{-i\omega_q t}$, we obtain $\tilde{w}(y,\omega_q) = w(y,-\omega_q)$ and

$$(v\partial_y - \omega_q) w(y,\omega_q) = ie\lambda_q(y) \ ,$$

which can easily be solved. For $y = D$, we finally get

$$\theta(t) = \sum_{q\neq 0} \left[w(-\omega_q) b_q^\dagger(t) + w(\omega_q) b_{-q}(t) \right] \ , \tag{18}$$

with

$$w(\omega_q) = (ie/v) \int_0^D dy\, \lambda_q(y) \exp[\omega_q (D-y)/v] \ . \tag{19}$$

Because of the associated dynamic image potential, the electron wave function acquires the phase factor $\exp[-i\theta(t)]$ during the tunneling process.

This effect can be properly incorporated by a modification of the tunneling Hamiltonian,

$$\tilde{H}_T = T\Psi^\dagger(0) e^{-i\theta} c_0 + \text{h.c.} \ . \tag{20}$$

The Greens function determining the effective TDOS is now given by

$$G(t) = \langle \exp[i\theta^\dagger(t)] \Psi(0,t) \Psi^\dagger(0,0) \exp[-i\theta(0)] \rangle \ . \tag{21}$$

Putting $G(t) = G_0(t)K(t)$, the contribution of the dynamic image potential then gives rise to the factor

$$K(t) = \exp[C_1(t) + C_2(t)] \ , \tag{22}$$

where we introduce the functions

$$\begin{aligned} C_1(t) &= -\frac{1}{2} \langle \theta^{\dagger 2}(t) + \theta^2(0) - 2\theta^\dagger(t)\theta(0) \rangle \ , \\ C_2(t) &= 2\pi \left[\langle \phi_p(t)\theta(0) \rangle + \langle \theta^\dagger(t)\phi_p(0) \rangle \right. \\ &\quad \left. - \langle \theta^\dagger(t)\phi_p(t) \rangle - \langle \phi_p(0)\theta(0) \rangle \right] , \end{aligned}$$

where C_2 is independent of $p = \pm$. Doing the Gaussian averages yields

$$C_1(t) = -\sum_{q\neq 0} [w(\omega_q)w(-\omega_q) + w^2(-\omega_q) \exp(-i\omega_q t)] \ , \tag{23}$$

$$C_2(t) = i(2\pi/L)^{1/2} \sum_{q\neq 0} \frac{w(-\omega_q)}{\sqrt{g(q)|q|}} [1 - \exp(-i\omega_q t)]. \tag{24}$$

Since we are interested in the power-law exponent governing the TDOS, we focus on the time-dependent parts of Eqs. (23) and (24), and do not explicitly compute the prefactor. For the interaction (1), numerical calculation of $K(t)$ gives the result shown in Fig. 2 which is well approximated by $|K(t)| = 1 + A(t)\cos(\Omega t)$ for long times, with oscillation frequency Ω. The amplitude decays according to $A(t) \propto t^{-\beta}$ with $\beta \approx 1.15$. This result is insensitive to the precise parameter values taken for $\xi, D/a$, and v/v_F. As a consequence, the *power-law exponent* α of the TDOS for small energy ϵ remains *unchanged by the dynamic image potential*. Hence one can indeed obtain the LL parameter g from a measurement of α.

This finding can be inferred analytically for a class of separable interaction potentials of the form

$$V(x,y) = V_0 \delta(x) f(y) \; , \tag{25}$$

where $f(y)$ is an arbitrary function with $f(D) = 1$. In this case, we get $\tilde{V}(q,y) = V_0 f(y)$, leading to $g(q) = g$. The time-dependent parts of Eqs. (23) and (24) read

$$C_1(t) \propto \int_0^\infty dq \; e^{-iv_F qt/g} q \left[\int_0^D dy \; f(y) e^{-v_F (D-y) q/gv} \right]^2 \; ,$$

$$C_2(t) \propto \int_0^\infty dq \; e^{-iv_F qt/g} \left[\int_0^D dy \; f(y) e^{-v_F (D-y) q/gv} \right] \; .$$

The asymptotic long-time behavior of $C_{1,2}(t)$ can be accurately calculated in stationary-phase approximation. We find that $C_1(t)$ decays faster than $1/t$, while $C_2(t) \propto 1/t$. Therefore, from Eq. (22), the TDOS exponent for small ϵ remains unchanged. We expect this result to be correct and generic for arbitrary physically relevant interaction potentials.

We conclude by summarizing our results. We have presented a simple theory of electron tunneling from a tip or a lead into a strongly correlated 1D metal, explicitly incorporating the finite traversal time and the dynamic response of the correlated metal to the incoming electron. We have solved this problem within a WKB-type approximation for different interaction potentials. Despite the presence of a strong static image potential, the power-law exponent entering the tunneling density of states is not affected by these effects, but completely determined by the correlation strength in the 1D metal.

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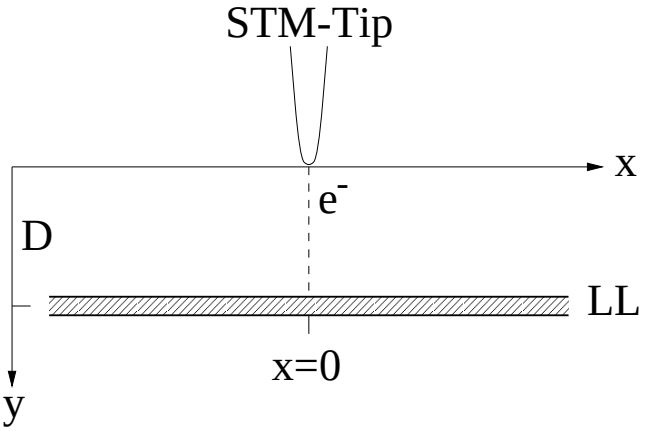

FIG. 1. Tunneling from an STM tip into a Luttinger liquid (schematic).

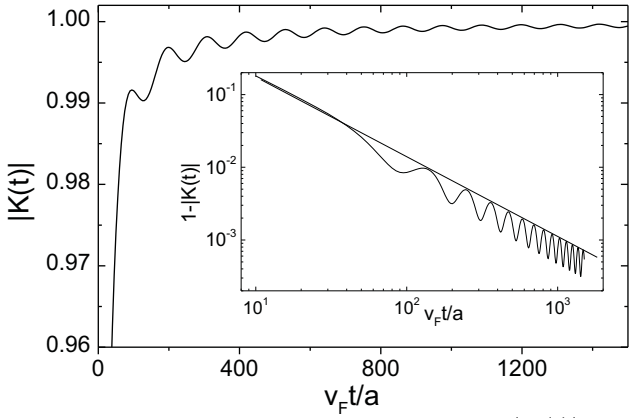

FIG. 2. Time-dependent correction factor $|K(t)|$ for the unscreened interaction (1). The parameter values are chosen as $\xi = 1.72$, $D/a = 3$, and $v/v_F = 1.48$. These values should be appropriate for nanotubes, where $U \approx 4$ eV and $v_F \approx 8 \times 10^5$ m/sec. The inset shows the decrease of the oscillation amplitude using double-logarithmic scales. The straight line is a guide to the eye only.